RESEARCH HIGHLIGHTS

Basic Energy Sciences Program Geosciences Subprogram

Project: Organic Anion - Mineral Surfaces

Who & Where: Patrick V. Brady, Randall, Randall T. Cygan, Kathryn L. Nagy Geochemistry Department, Sandia National Laboratories, Albuquerque, NM 87185-0750 (505-844-5337; FAX 844-7146) EMAIL pvbrady@sandia.gov

Objective: The general focus of this project is mineral surface geochemistry. The specific focus is organic acid interactions with mineral surfaces.

Results: Kaolinite is an ideal mineral for studying the fundamental origins of multi-oxide silicate surface charge. The chemical reactivities of exposed tetrahedral Si and hydrated octahedral Al groups might approximate the chemical behavior of the same groups exposed on more complex aluminosilicate minerals. Nevertheless, the site-specific origins of kaolinite surface charge and its absolute magnitude remain a matter of debate. Brady, Cygan, and Nagy approached the problem from three different directions and used potentiometric titrations (Figure 1), molecular modeling calculations (Figure 2), and imaging by scanning force microscopy to examine both questions.

Significance: The results, soon to be published in the Journal of Colloid and Interface Science, point to control of kaolinite surface charge by highly acid Al sites below about pH 8 (At higher pH deprotonated Si sites contribute to the total charge). The acidity of Al sites exposed at kaolinite edges is much greater than that on pure Al oxides. Si sites on kaolinite edges have roughly the same acidity as those on pure Si minerals, such as quartz. At the same time, edge sites make up a larger proportion (20-40%) of the total accessible surface than generally believed.

Publication: A journal article entitled "Molecular Controls on Kaolinite Surface Charge" has been written by Brady P. V., R. T. Cygan, and K. L. Nagy (Journal of Colloid and Interface Science, in press).

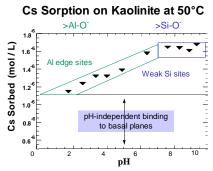


Figure 1. Potentiometric Titrations

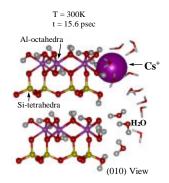


Figure 2. Molecular Modeling of Cs Sorption